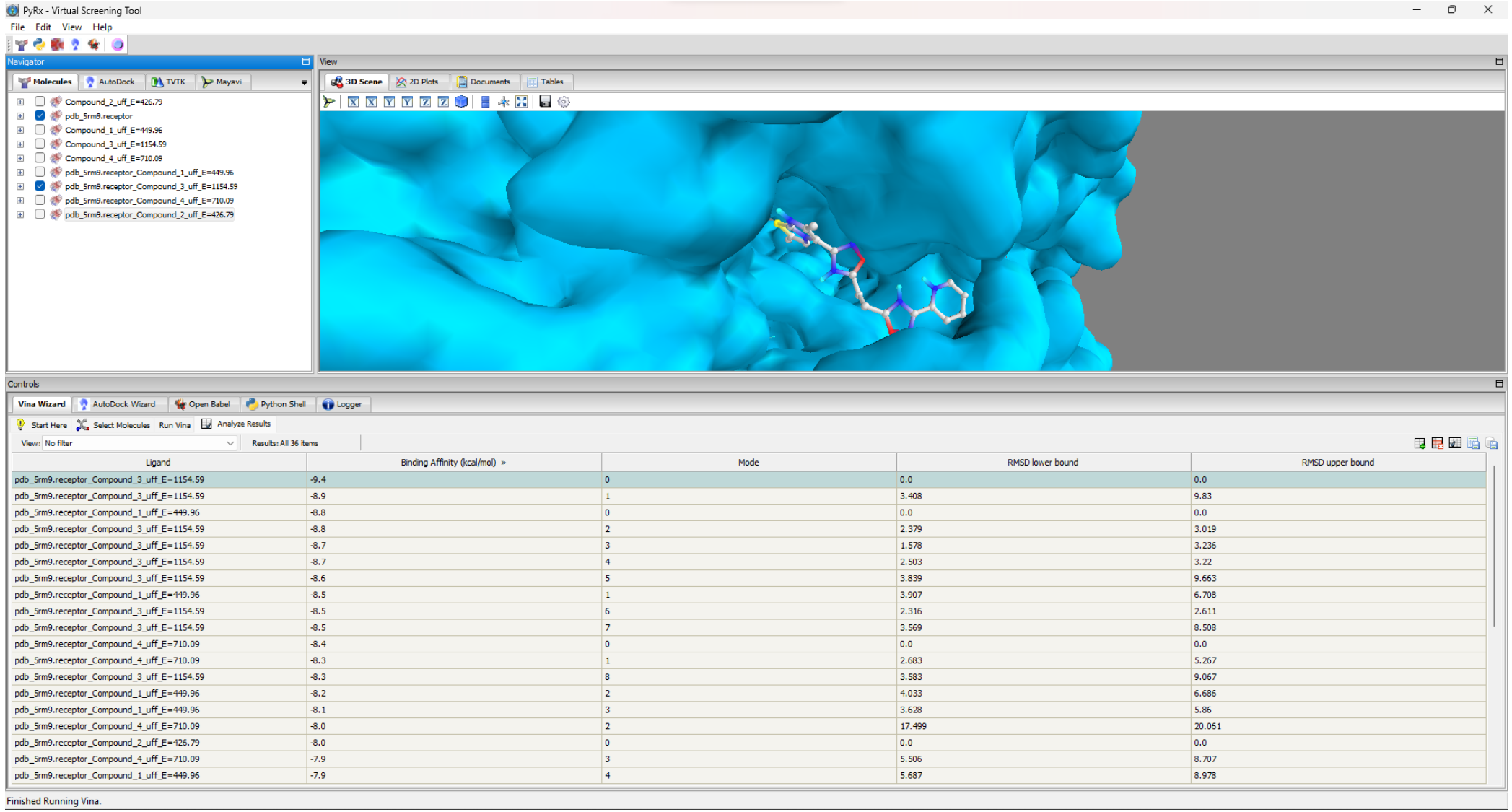
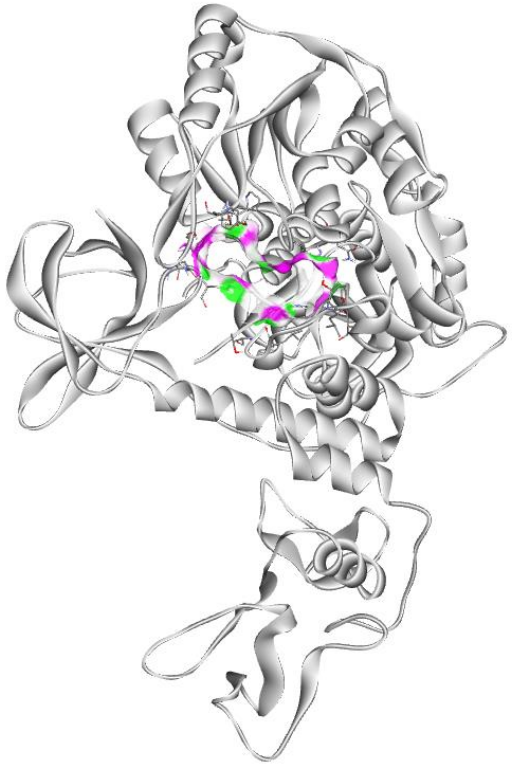
PyRx/ AutoDock VINA Virtual Screen:
DEL Unwindase compounds

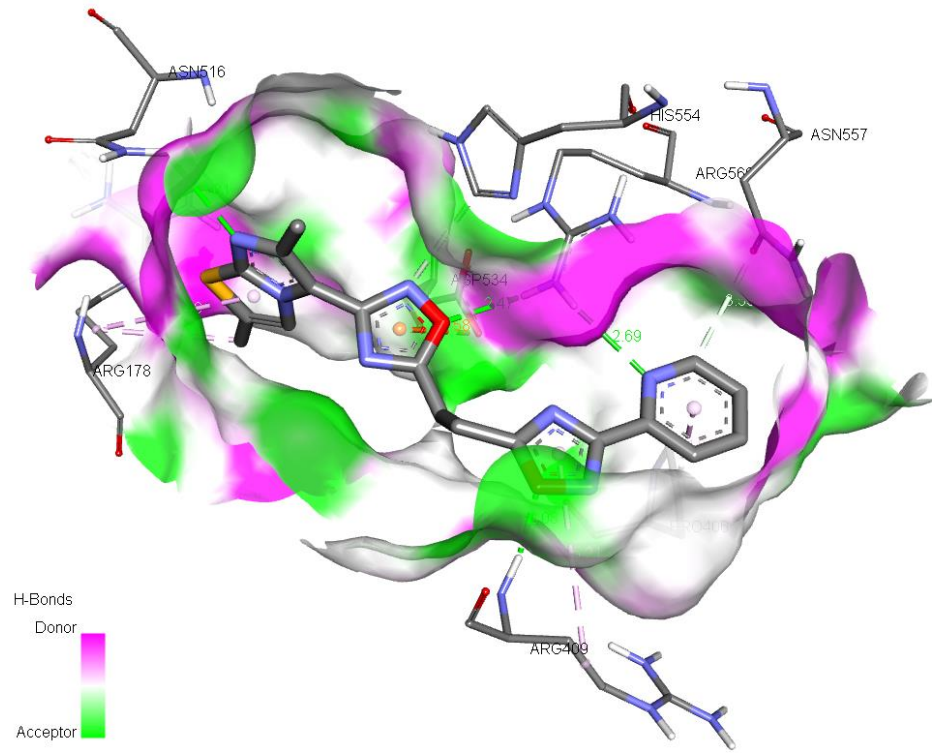


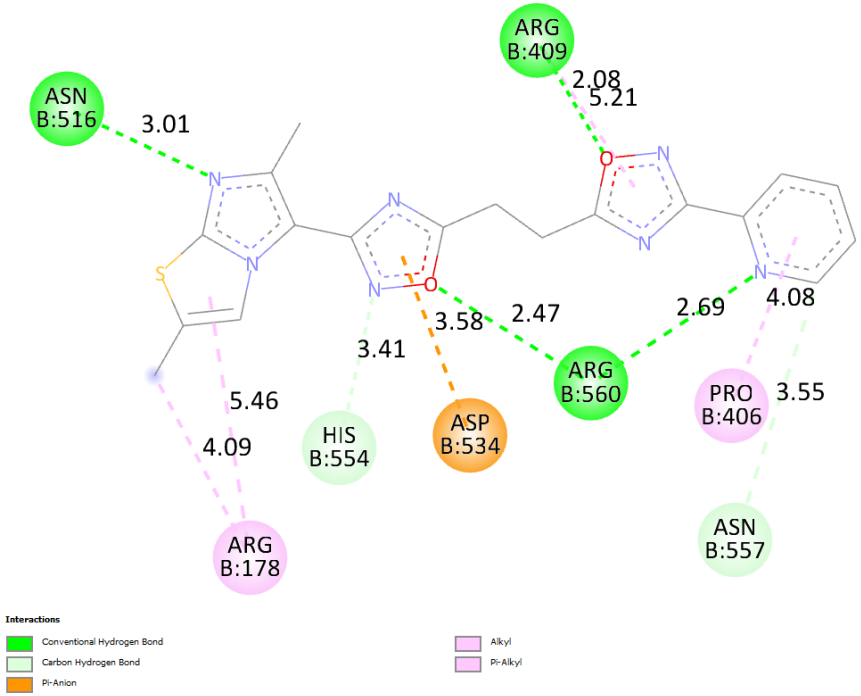
Ligand	Binding Affinity (kcal/mol)	Mode	RMSD lower bound	RMSD upper bound
pdb_5rm9.receptor_Compound_3_uff_E=1154.59	-9.4	0	0.0	0.0
pdb_5rm9.receptor_Compound_3_uff_E=1154.59	-8.9	1	3.408	9.83
pdb_5rm9.receptor_Compound_1_uff_E=449.96	-8.8	0	0.0	0.0
pdb_5rm9.receptor_Compound_3_uff_E=1154.59	-8.8	2	2.379	3.019
pdb_5rm9.receptor_Compound_3_uff_E=1154.59	-8.7	3	1.578	3.236
pdb_5rm9.receptor_Compound_3_uff_E=1154.59	-8.7	4	2.503	3.22
pdb_5rm9.receptor_Compound_3_uff_E=1154.59	-8.6	5	3.839	9.663
pdb_5rm9.receptor_Compound_1_uff_E=449.96	-8.5	1	3.907	6.708
pdb_5rm9.receptor_Compound_3_uff_E=1154.59	-8.5	6	2.316	2.611
pdb_5rm9.receptor_Compound_3_uff_E=1154.59	-8.5	7	3.569	8.508
pdb_5rm9.receptor_Compound_4_uff_E=710.09	-8.4	0	0.0	0.0
pdb_5rm9.receptor_Compound_4_uff_E=710.09	-8.3	1	2.683	5.267
pdb_5rm9.receptor_Compound_3_uff_E=1154.59	-8.3	8	3.583	9.067
pdb_5rm9.receptor_Compound_1_uff_E=449.96	-8.2	2	4.033	6.686
pdb_5rm9.receptor_Compound_1_uff_E=449.96	-8.1	3	3.628	5.86
pdb_5rm9.receptor_Compound_4_uff_E=710.09	-8.0	2	17.499	20.061
pdb_5rm9.receptor_Compound_2_uff_E=426.79	-8.0	0	0.0	0.0
pdb_5rm9.receptor_Compound_4_uff_E=710.09	-7.9	3	5.506	8.707
pdb_5rm9.receptor_Compound_1_uff_E=449.96	-7.9	4	5.687	8.978

RA-0003509-01

- Minimum binding free energy = -9.4 kcal/mol
- DEL Screen: 72%inhibition at 20 mM

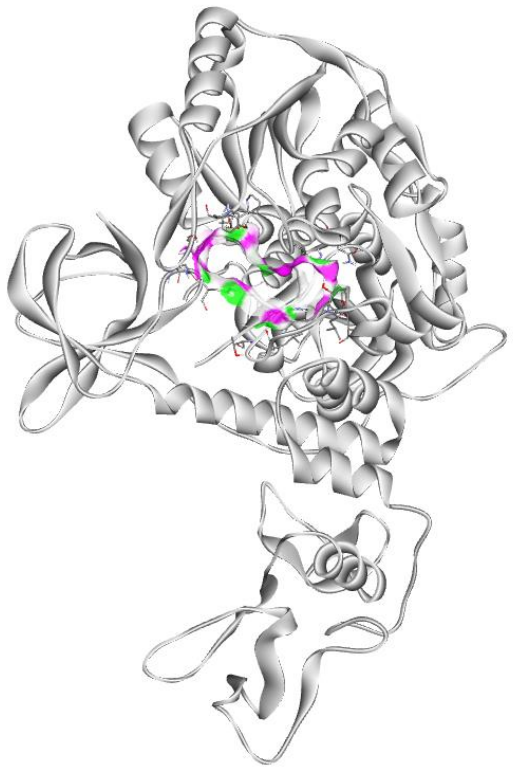


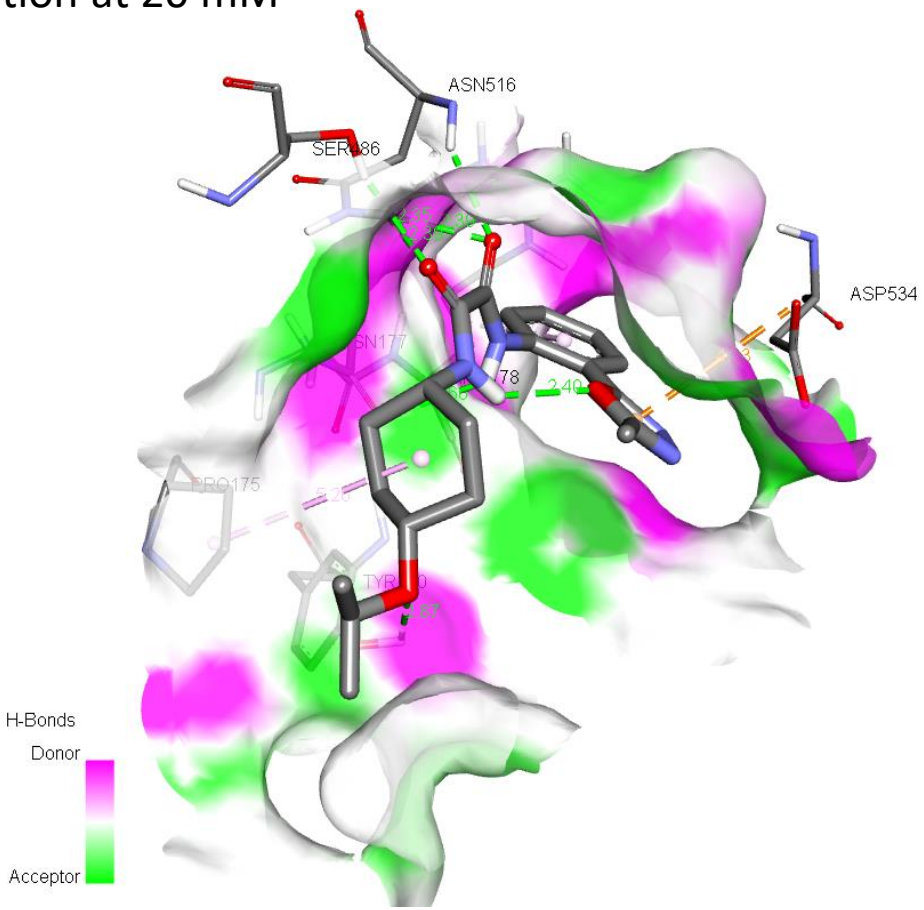


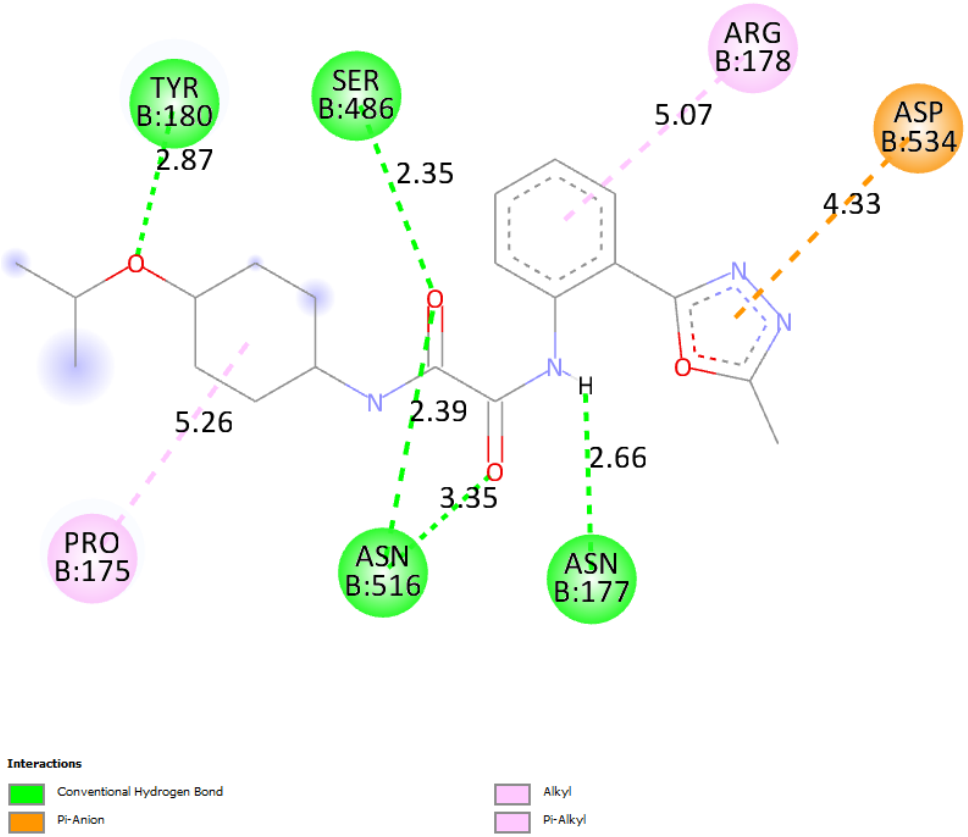


RA-0003491-01

- Minimum binding free energy = -8.8 kcal/mol
- DEL Screen: 89%inhibition at 20 mM

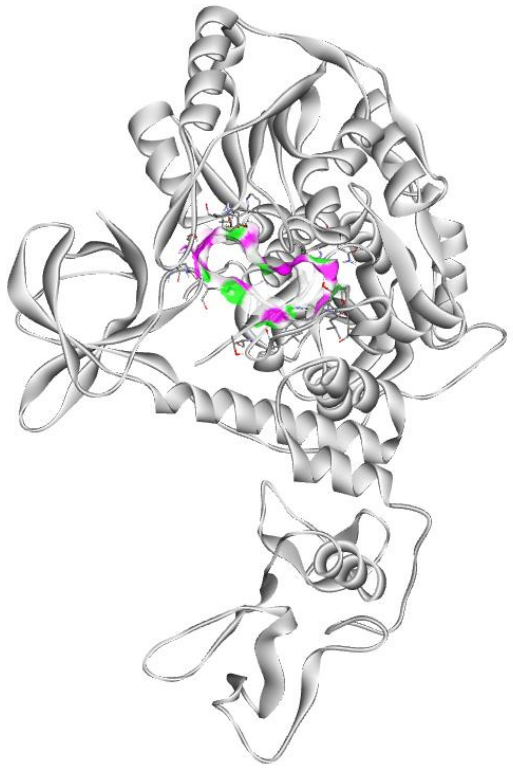


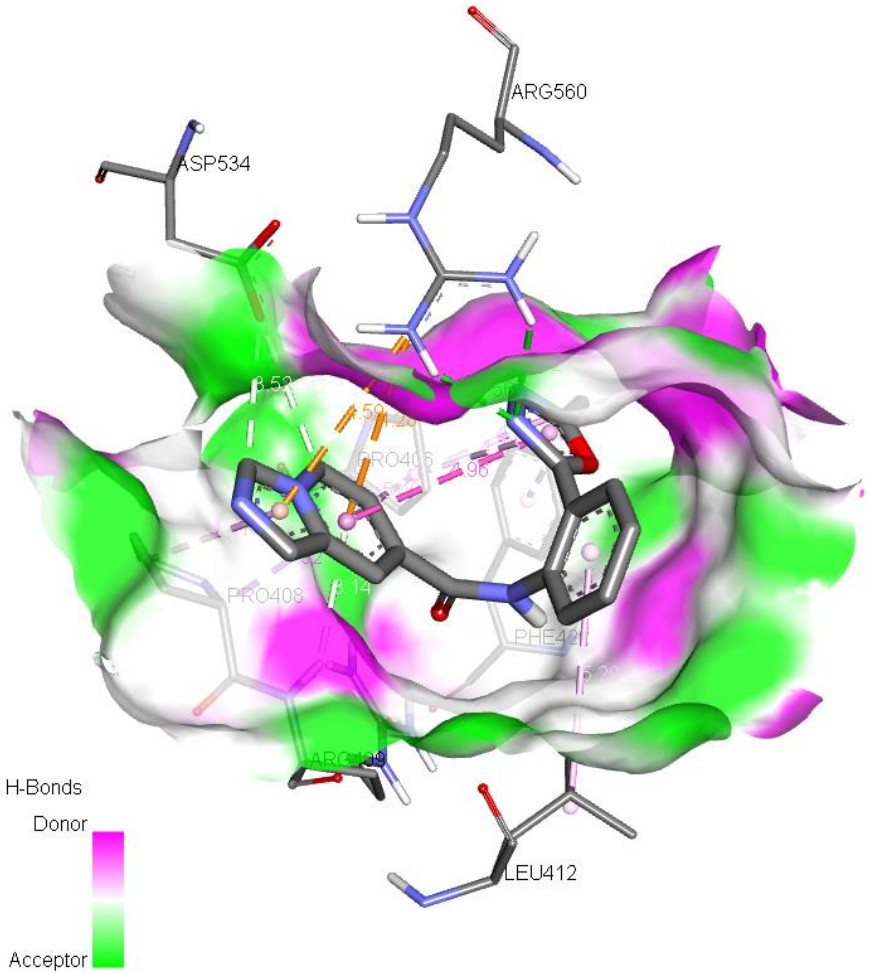


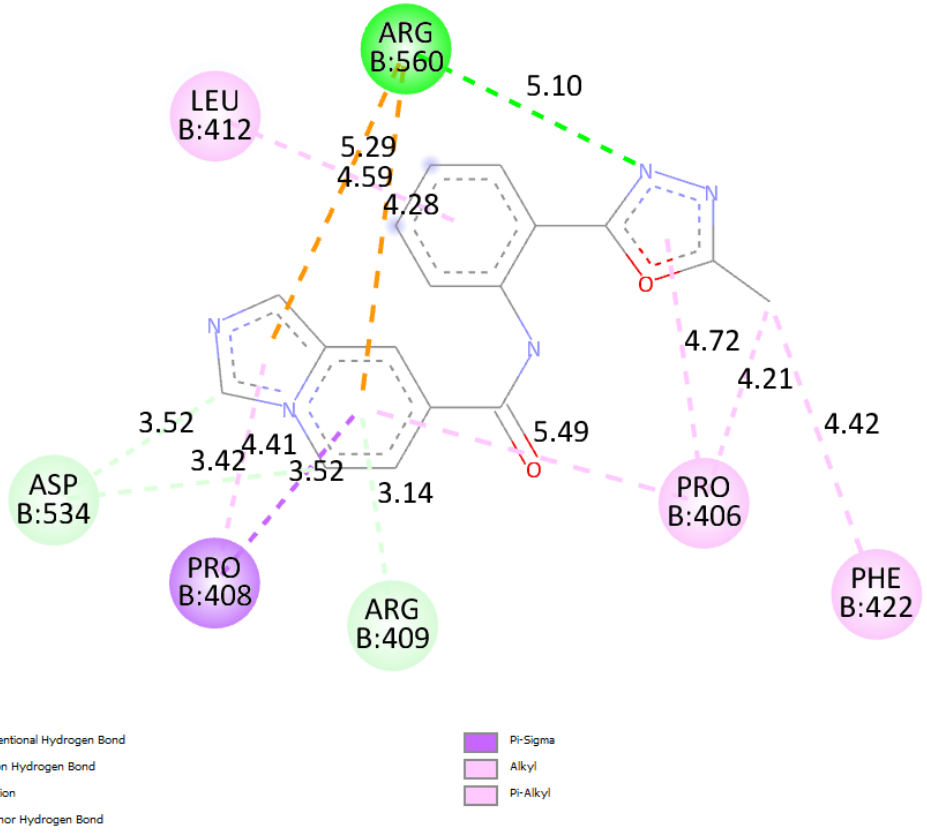


RA-0003487-01

- Minimum binding free energy = -8.4 kcal/mol
- DEL Screen: 50%inhibition at 20 mM







RA-0003439-01

- Minimum binding free energy = -8.8 kcal/mol
- DEL Screen: 82%inhibition at 20 mM